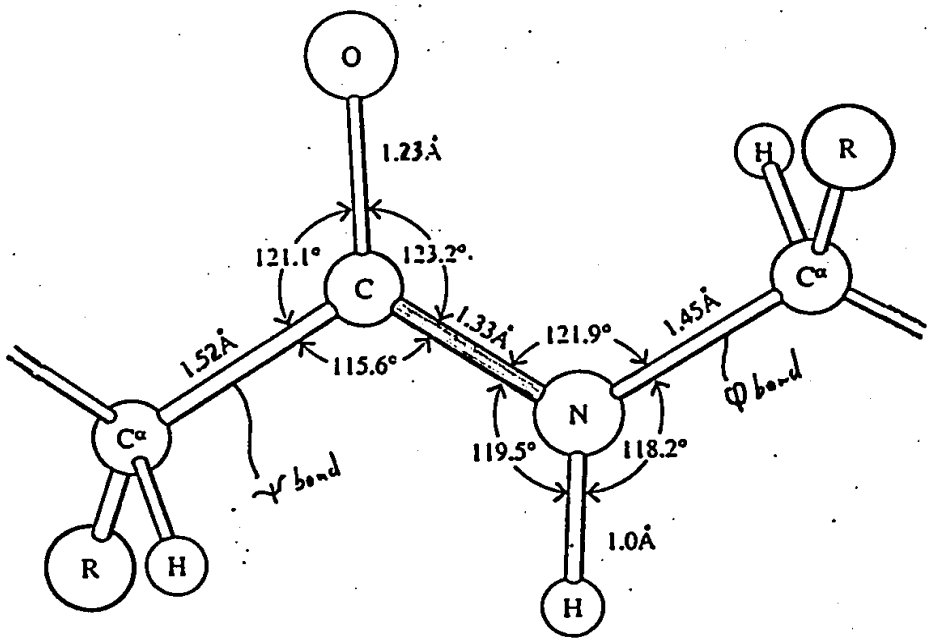

O
1.23Å
121.1°
123.2°
C
1.33Å
121.9°
1.45Å
H
R
Cα
1.52Å
115.6°
Cα
N
ψ bond
φ bond
119.5°
118.2°
1.0Å
R
H
H

Fig. 1

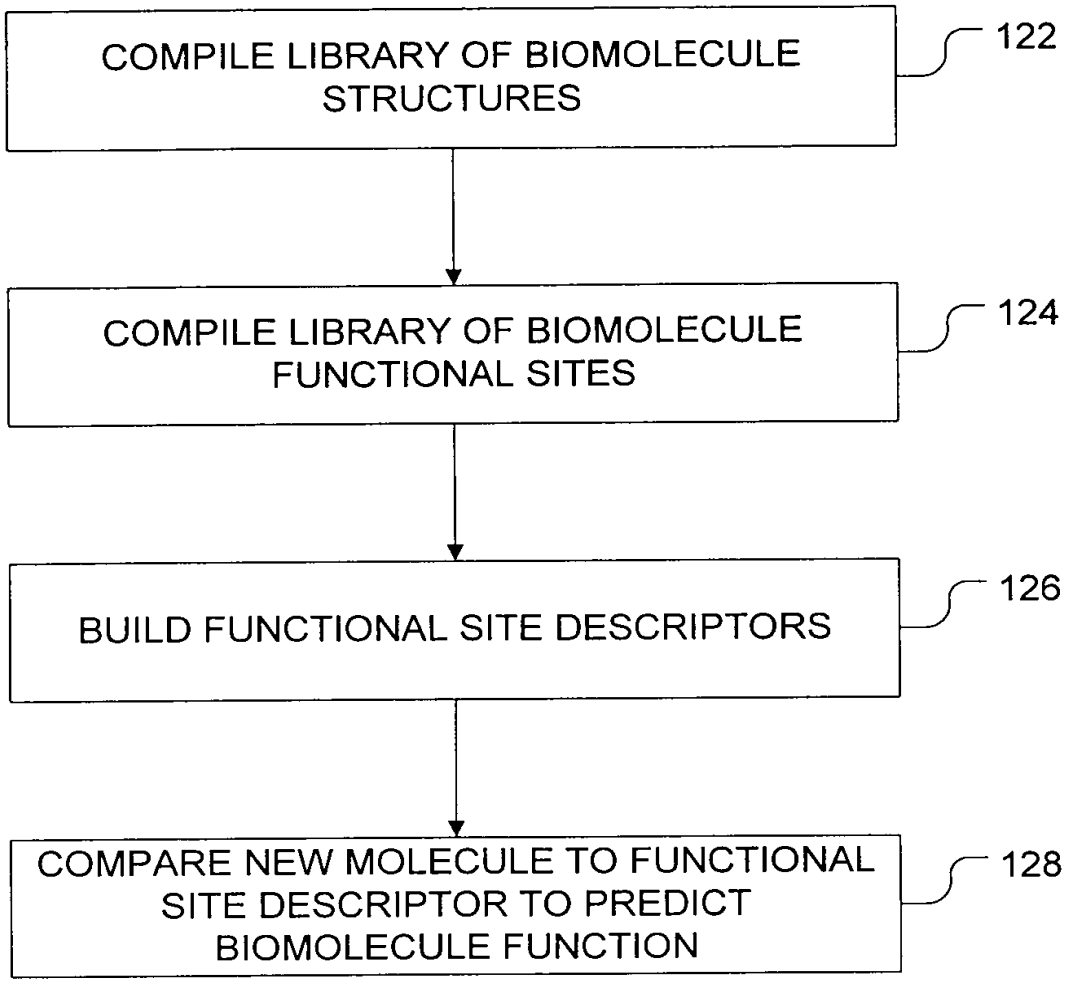
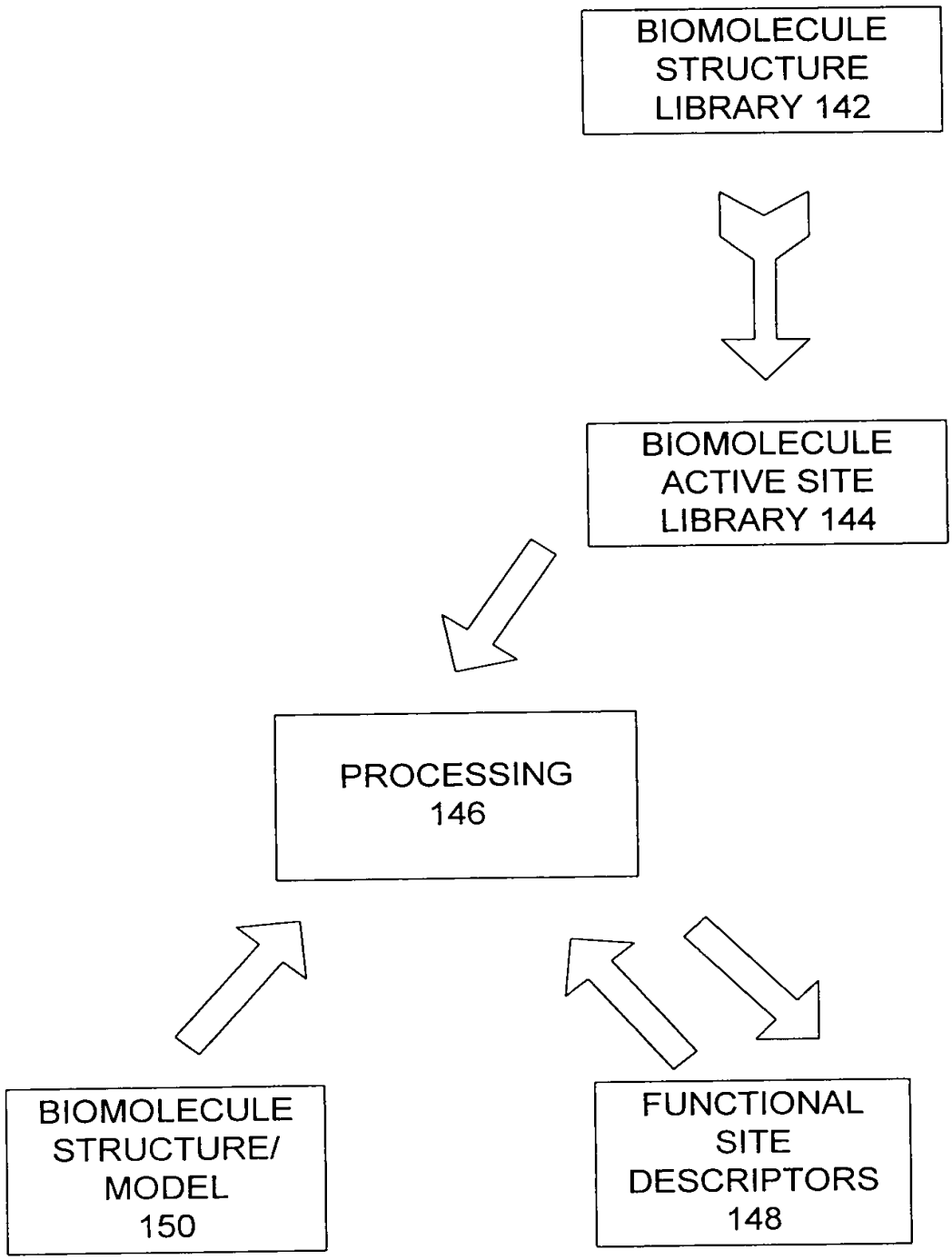

COMPILE LIBRARY OF BIOMOLECULE STRUCTURES
122
COMPILE LIBRARY OF BIOMOLECULE FUNCTIONAL SITES
124
BUILD FUNCTIONAL SITE DESCRIPTORS
126
COMPARE NEW MOLECULE TO FUNCTIONAL SITE DESCRIPTOR TO PREDICT BIOMOLECULE FUNCTION
128

Fig. 2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BIOMOLECULE ACTIVE SITE LIBRARY 144
PROCESSING 146
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Fig. 3

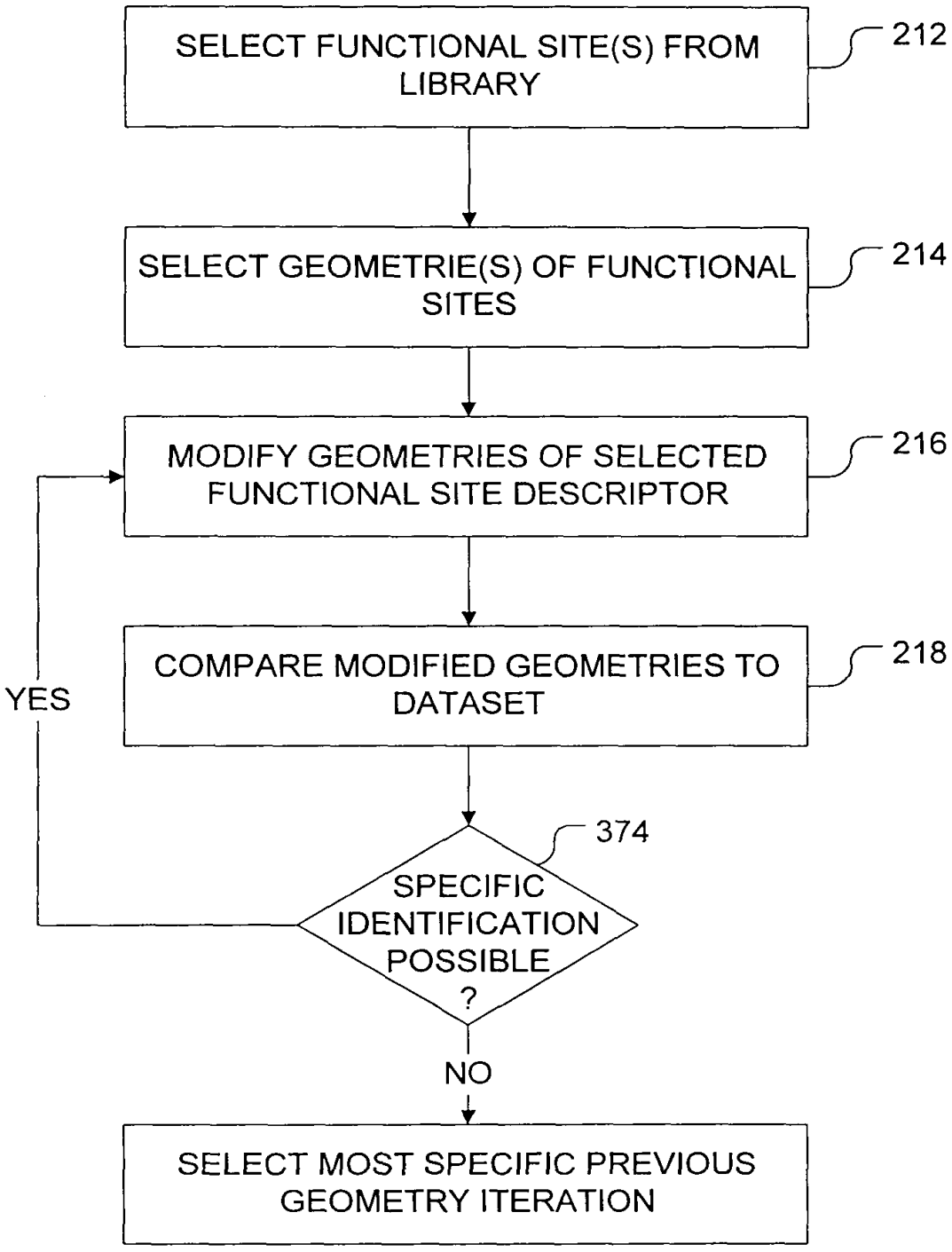

SELECT FUNCTIONAL SITE(S) FROM LIBRARY
212
SELECT GEOMETRIE(S) OF FUNCTIONAL SITES
214
MODIFY GEOMETRIES OF SELECTED FUNCTIONAL SITE DESCRIPTOR
216
COMPARE MODIFIED GEOMETRIES TO DATASET
218
374
SPECIFIC IDENTIFICATION POSSIBLE ?
YES
NO
SELECT MOST SPECIFIC PREVIOUS GEOMETRY ITERATION

Fig. 4

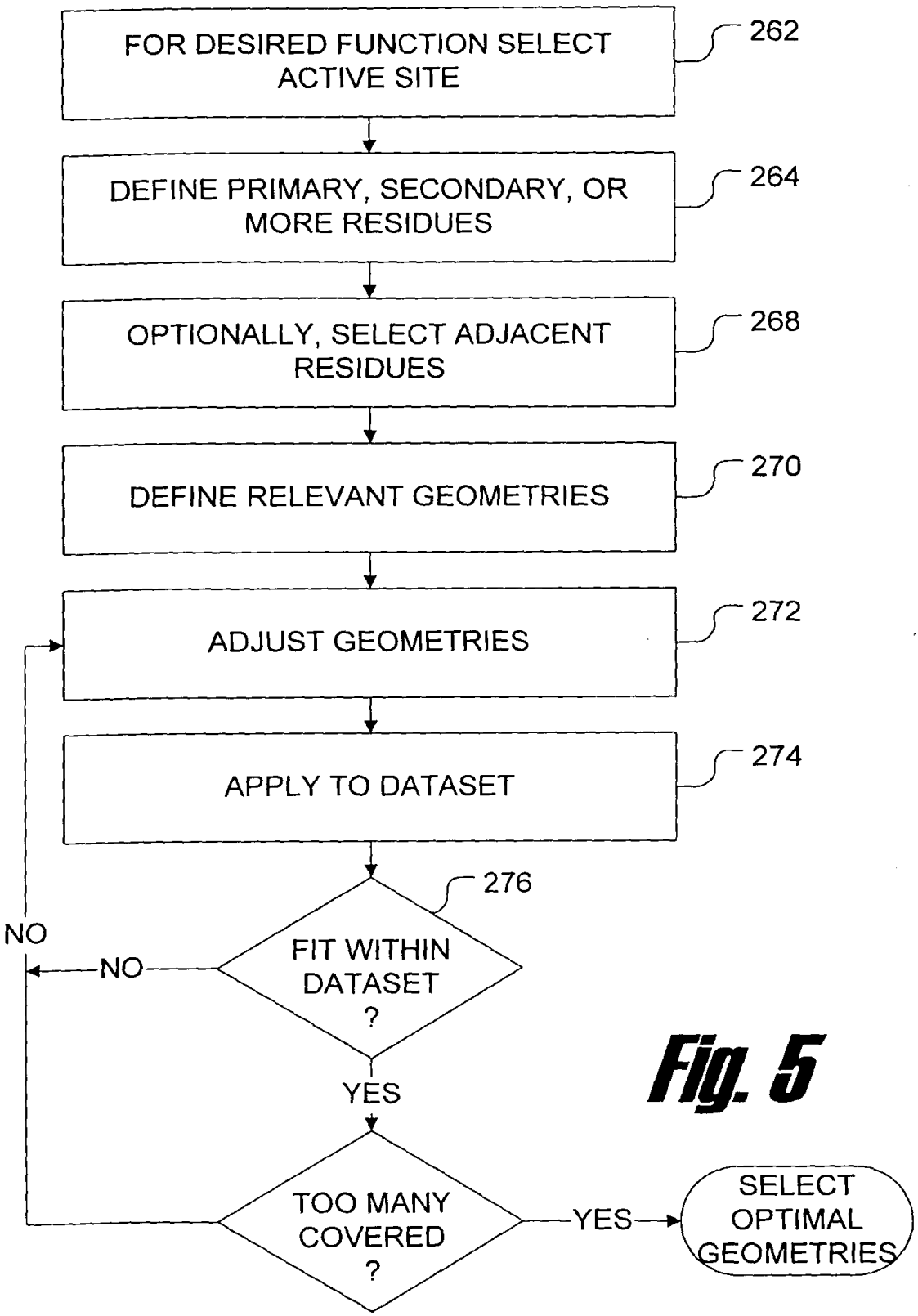
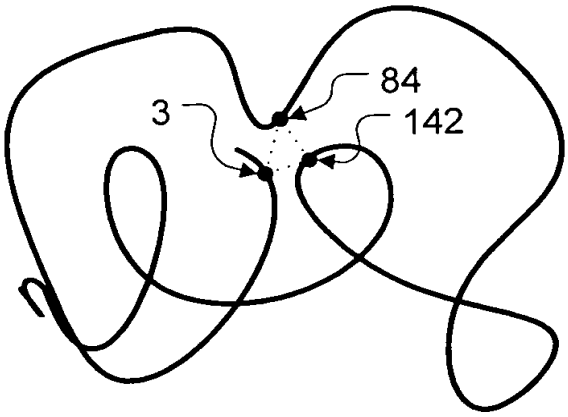

FOR DESIRED FUNCTION SELECT ACTIVE SITE
262
DEFINE PRIMARY, SECONDARY, OR MORE RESIDUES
264
OPTIONALLY, SELECT ADJACENT RESIDUES
268
DEFINE RELEVANT GEOMETRIES
270
ADJUST GEOMETRIES
272
APPLY TO DATASET
274
276
FIT WITHIN DATASET ?
NO
NO
YES
TOO MANY COVERED ?
YES
SELECT OPTIMAL GEOMETRIES

Fig. 5

Fig. 6A



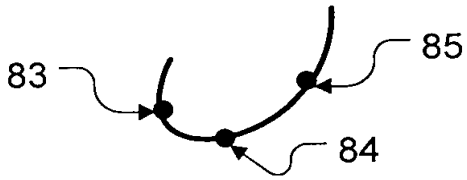
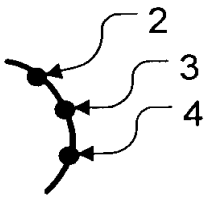


Fig. 6B



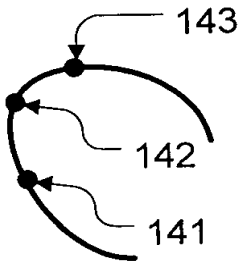
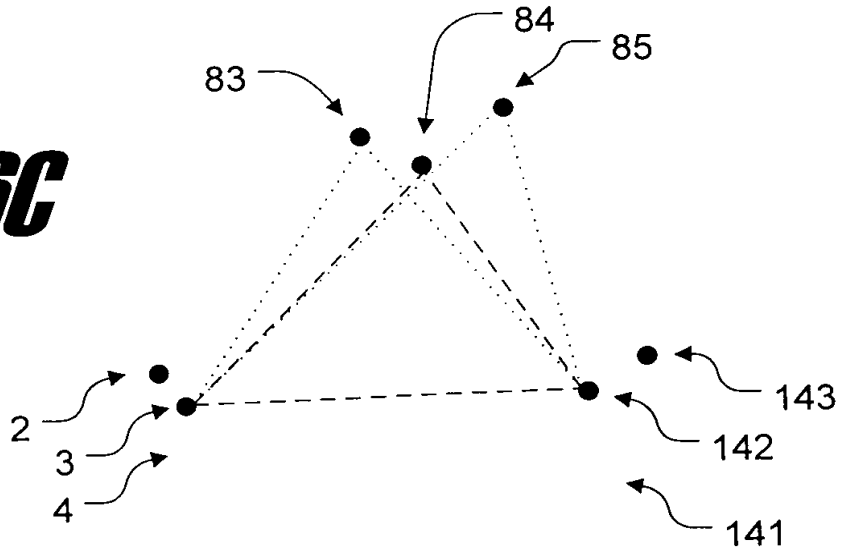


Fig. 6C



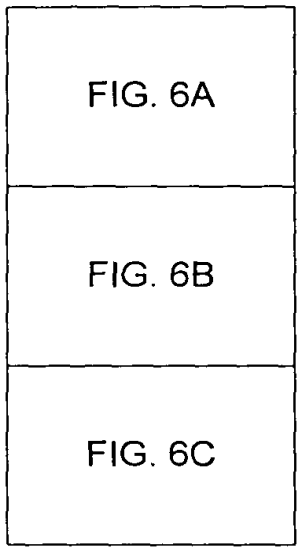


FIG. 6A
FIG. 6B
FIG. 6C

Fig. 6

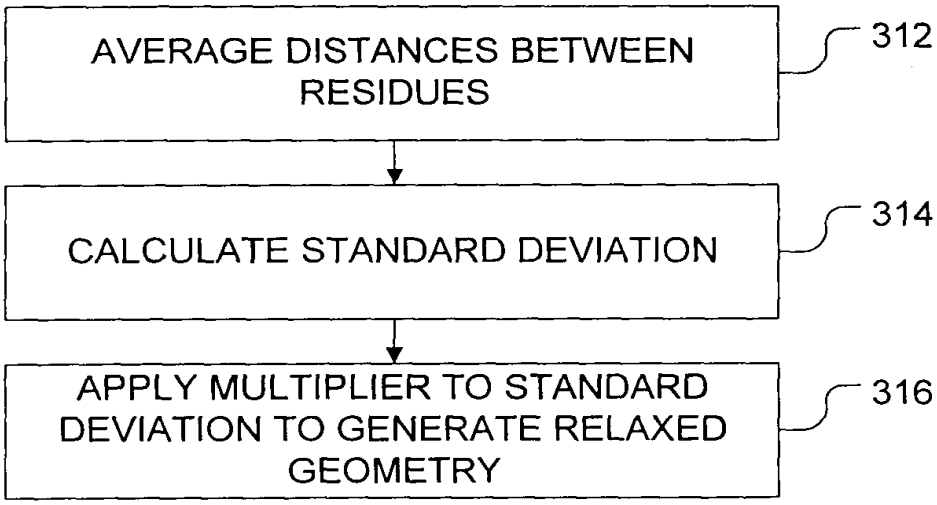

AVERAGE DISTANCES BETWEEN RESIDUES
312
CALCULATE STANDARD DEVIATION
314
APPLY MULTIPLIER TO STANDARD DEVIATION TO GENERATE RELAXED GEOMETRY
316

Fig. 7

	AVE DIST 322	STD DEV 324	MULT 326
A→B	3.83	0.03	2.0
B→C	10.09	0.14	2.0
A→C	7.2	0.09	2.0
A-1→B	5.46	0.04	2.0
A+1→B	0.00	0.00	2.0
C-1→A	6.05	0.10	2.0
C+1→A	9.63	0.06	2.0
B-1→A	0.00	0.00	2.0
B+1→A	5.38	0.09	2.0

Fig. 8

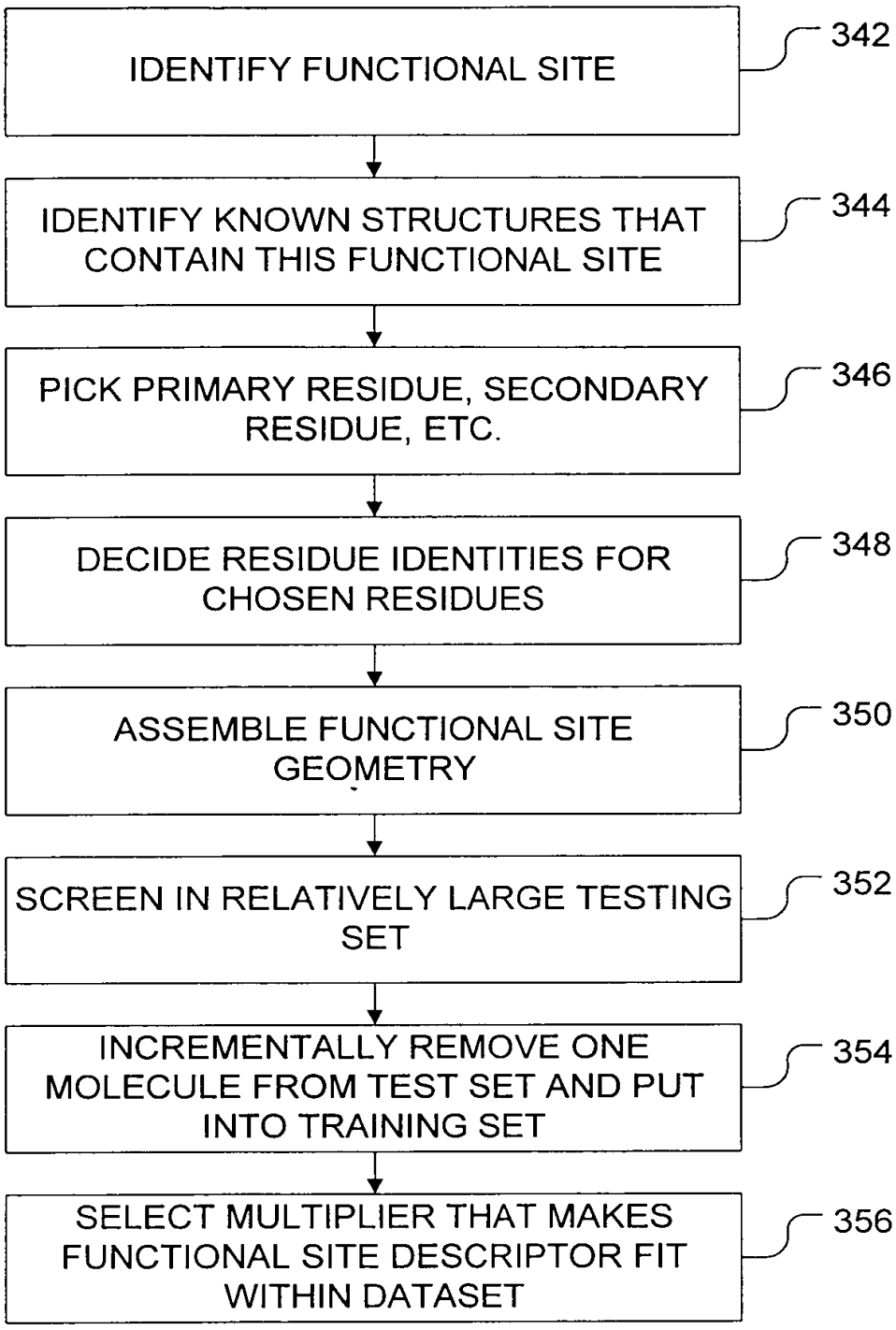

IDENTIFY FUNCTIONAL SITE
342
IDENTIFY KNOWN STRUCTURES THAT CONTAIN THIS FUNCTIONAL SITE
344
PICK PRIMARY RESIDUE, SECONDARY RESIDUE, ETC.
346
DECIDE RESIDUE IDENTITIES FOR CHOSEN RESIDUES
348
ASSEMBLE FUNCTIONAL SITE GEOMETRY
350
SCREEN IN RELATIVELY LARGE TESTING SET
352
INCREMENTALLY REMOVE ONE MOLECULE FROM TEST SET AND PUT INTO TRAINING SET
354
SELECT MULTIPLIER THAT MAKES FUNCTIONAL SITE DESCRIPTOR FIT WITHIN DATASET
356

Fig. 9

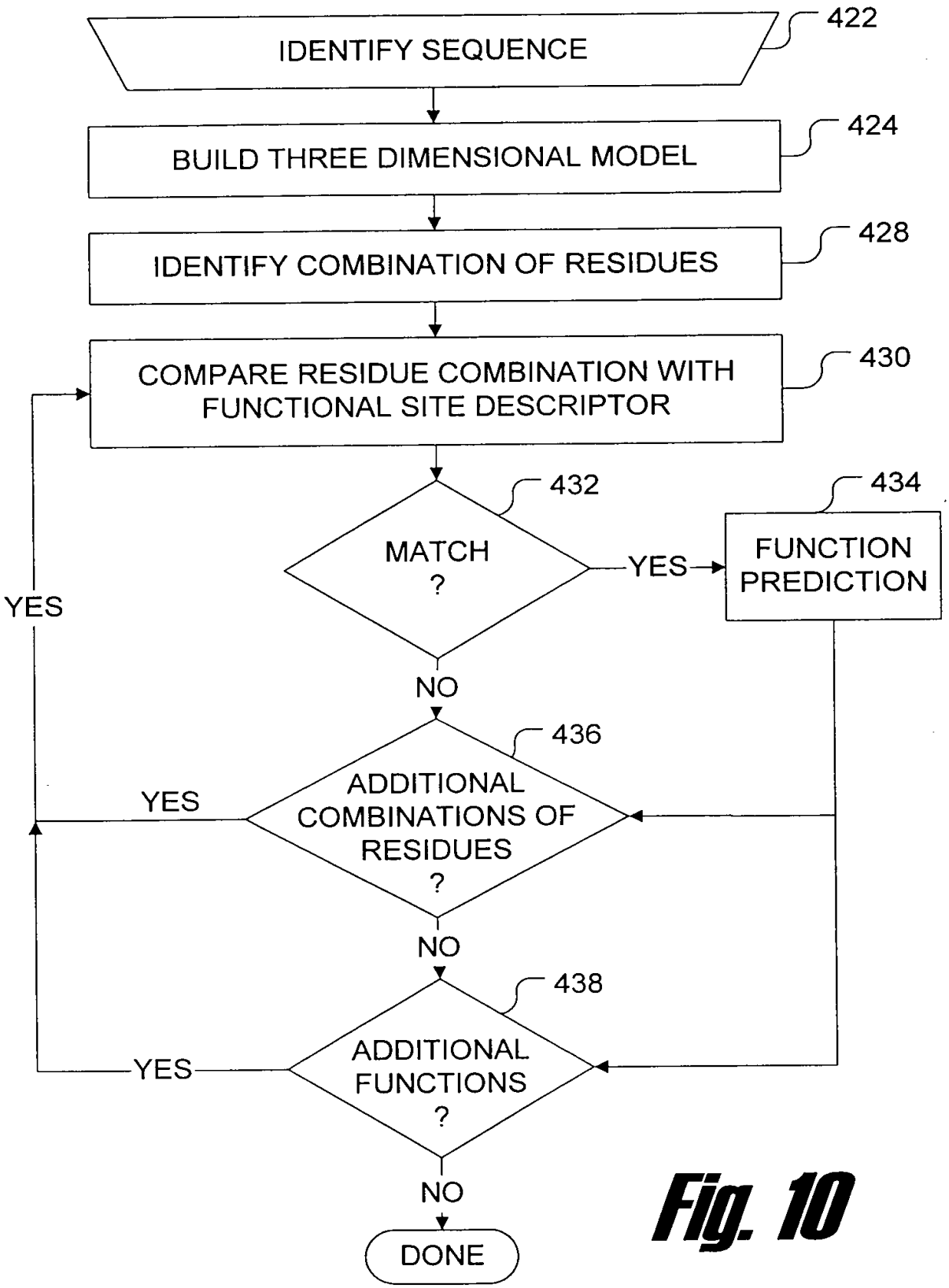

IDENTIFY SEQUENCE
422
BUILD THREE DIMENSIONAL MODEL
424
IDENTIFY COMBINATION OF RESIDUES
428
COMPARE RESIDUE COMBINATION WITH FUNCTIONAL SITE DESCRIPTOR
430
MATCH ?
432
YES
FUNCTION PREDICTION
434
YES
NO
ADDITIONAL COMBINATIONS OF RESIDUES ?
436
YES
NO
ADDITIONAL FUNCTIONS ?
438
YES
NO
DONE

Fig. 10

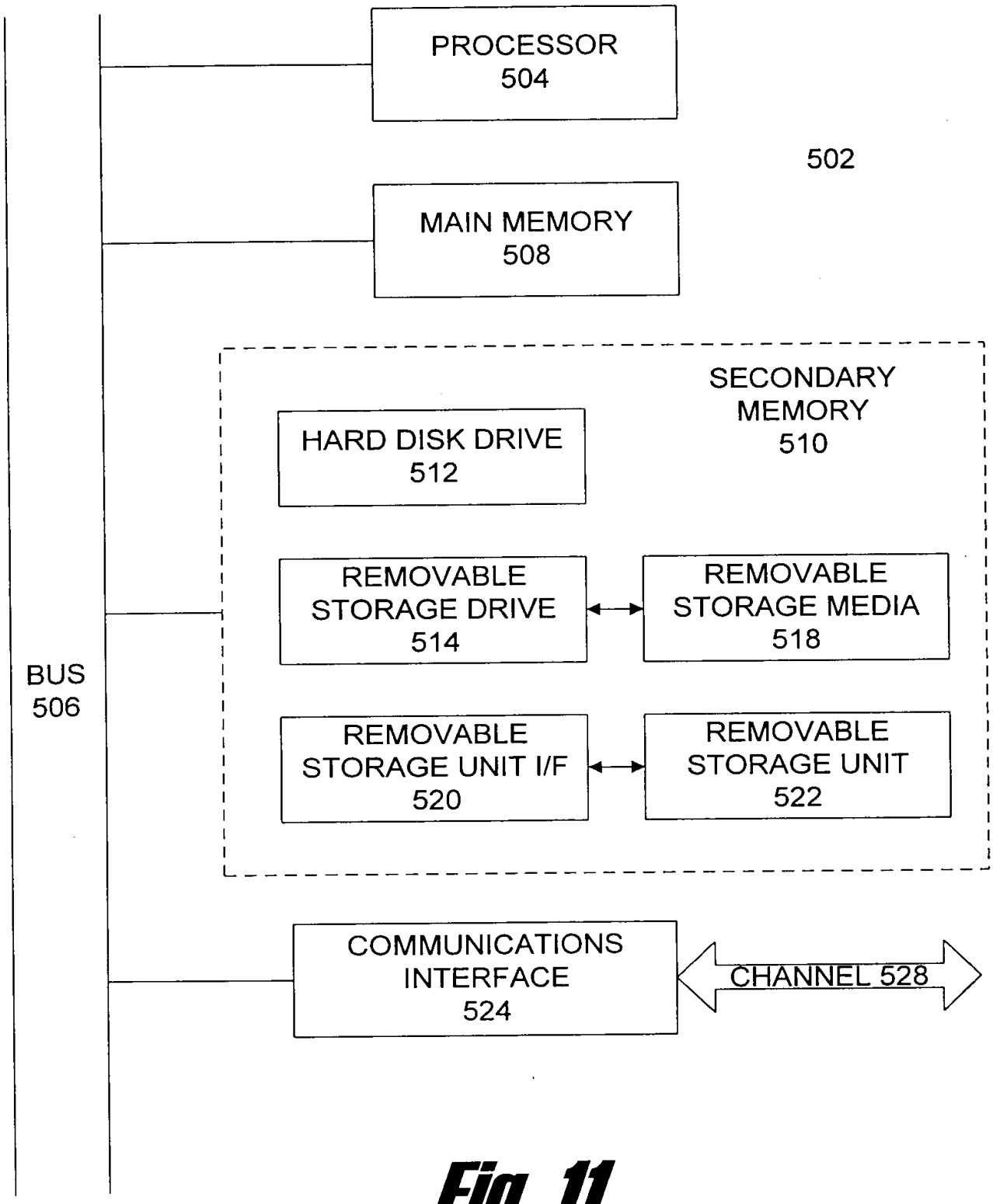

PROCESSOR
504
502
MAIN MEMORY
508
SECONDARY
MEMORY
510
HARD DISK DRIVE
512
REMOVABLE
STORAGE DRIVE
514
REMOVABLE
STORAGE MEDIA
518
BUS
506
REMOVABLE
STORAGE UNIT I/F
520
REMOVABLE
STORAGE UNIT
522
COMMUNICATIONS
INTERFACE
524
CHANNEL 528

Fig. 11

```
          1                                                        50
RNT1_ASPOR ..........  ...MMYSKLL TLTTLLLPTA LALPSLVERA CDYTCGSNCY
RNF1_FUSMO ..........  .......... .......... .........Q SATTCGSTNY
RNMS_ASPSA ..........  .......... .......... .........ES CEYTCGSTCY
RNU2_USTSP ..........  .......... .......... .......CNIP ESTNCGGNVY
RNC2_ASPCL ..........  .......... .......... .........D CDYTCGSHCY
RNPB_PENBR ..........  .......... .......... .........A CAATCGTVCY
RNPC_PENCH ..........  .......... .......... .........A CAATCGSVCY
RNN1_NEUCR ..........  .......... .......... .........A CMYICGSVCY
RNU1_USTSP ..........  .......... .......... .........QGG VSVNCGGTYY
RNAS_ASPGI MVAIKNLVLV ALTAVTALAV PSPLEARAVT WTCLNDQKNP KTNKYETKRL
RNCL_ASPCL MVAIKNLVLV ALTAVTALAM PSPLEERAAT WTCMNEQKNP KTNKYENKRL
RNMG_ASPRE MVAIKNLFLL AATAVSVLAA PSPLDARA.T WTCINQQLNP KTNKWEDKRL

          51                                                      100
RNT1_ASPOR SSSDVSTAQA AGYQLHEDGE TVGSNSYPHK YNN.YEG... .......FDF
RNF1_FUSMO SASQVRAAAN AACQYYQNDD SAGSTTYPHT YNN.YEG... .......FDF
RNMS_ASPSA WSSDVSAAKA KGYSLYESGD TI..DDYPHG YHD.YEG... .......FDF
RNU2_USTSP SNDDINTAIQ GA...LDDVA RPDGDNYPHQ YYD.EAS... .......EDI
RNC2_ASPCL SASAVSDAQS AGYQLESAGQ SVGRSRYPHQ YRN.YEG... .......FNF
RNPB_PENBR TSSAISSAQA AGYNLYSTND DV..SNYPHE YHN.YEG... .......FDF
RNPC_PENCH TSSAISAAQE AGYDLYSAND DV..SNYPHE YRN.YEG... .......FDF
RNN1_NEUCR SSSAISAALN KGYSYYEDGA TAGSSSYPHR YNN.YEG... .......FDF
RNU1_USTSP SSTQVNRAIN NA.....KSG QYSSTGYPHT YNN.YEG... .......FDF
RNAS_ASPGI LYNQNKAESN SHHAPLSDGK T..GSSYPHW FTNGYDGDGK LPKGRTPIKF
RNCL_ASPCL LYNQNNAESN AHHAPLSDGK T..GSSYPHW FTNGYDGDGK ILKGRTPIKW
RNMG_ASPRE LYSQAKAESN SHHAPLSDGK T..GSSYPHW FTNGYDGNGK LIKGRTPIKF

          101                                                     150
RNT1_ASPOR ..S.VSSP..  .......... ..YYEWPILS SGDVYS..G. ...GSPGADR
RNF1_FUSMO ..P.VDGP..  .......... ..YQEPPIKS GG.VYT..G. ...GSPGADR
RNMS_ASPSA ..P.VSGT..  .......... ..YYEYPIMS DYDVYT..G. ...GSPGADR
RNU2_USTSP TLCCGPGS..  .......... ..WSEPPLVY NGPYYS..SR DNYVSPGPDR
RNC2_ASPCL ..P.VSGN..  .......... ..YYENPILS SGSTYN..G. ...GGPGADR
RNPB_PENBR ..P.VSGT..  .......... ..YYEPPILK SGKVYT..G. ...SSPGADR
RNPC_PENCH ..P.VSGT..  .......... ..YYEPPILR SGAVYS..G. ...NSPGADR
RNN1_NEUCR ..P.TAKP..  .......... ..WYEPPILS SGRVYT..G. ...GSPGADR
RNU1_USTSP S.DYCDGP..  .......... ..YKEYPLKT SSSGYT..G. ...GSPGADR
RNAS_ASPGI GKSDCDRPPK HSKDGNGKTD HYLLEPPTPP DGHDYKFDSK KPKENPGPAR
RNCL_ASPCL GNSDCDRPPK HSKNGDGKND HYLLEPPTPP DGHQYNFDSK KPKEDPGPAR
RNMG_ASPRE GKADCDRPPK HSQNGMGKDD HYLLEPPTPP DGHDYKFDSK KPKEDPGPAR

          151                                  182
RNT1_ASPOR VVFNENNQ.L AGVITHTGAS G.NNFVECT. ..
RNF1_FUSMO VVINTNCE.Y AGAITHTGAS G.NNFVGCSG TN
RNMS_ASPSA VIFNGDDE.L AGVITHTGAS G.DDFVACSS S.
RNU2_USTSP VIYQTNTGEF CATVTHTGAA SYDGFTQCS. ..
RNC2_ASPCL VVFNDNDE.L AGLITHTGAS G.DGFVACY. ..
RNPB_PENBR VIFNDDDE.L AGVITHTGAS G.NNFVACT. ..
RNPC_PENCH VVFNGNDQ.L AGVITHTGAS G.NNFVACD. ..
RNN1_NEUCR VIFDSHGN.L DMLITHNGAS G.NNFVACN. ..
RNU1_USTSP VVYDSNDGTF CGAITHTGAS G.NNFVQCSY ..
RNAS_ASPGI VIYTYPNKVF CGIIAHTKEN Q.GELKLCSH ..
RNCL_ASPCL VIYTYPNKVF CGIVAHTREN Q.GDLKLCSH ..
RNMG_ASPRE VIYTYPNKVF CGIVAHQRGN Q.GDLRLCSH ..
```

Fig. 12/1

		1rtu	1fus	1rms	AVG	SD	Actual	Var	9mt
30s His	90sHis	15.20	16.70	15.97	15.950	0.6577	15.9	1.5	15.63
30s His	Glu	5.36	5.84	5.71	5.637	0.2221	5.7	0.5	5.79
90s His	Glu	13.03	12.90	12.44	12.580	0.2773	12.6	1.0	11.95
Tyr	Phe	16.69	16.40	16.62	16.580	0.1290	16.5	0.5	16.43
Tyr	Arg	10.50	10.20	10.25	10.330	0.1473	10.3	0.5	10.29
Phe	Arg	9.61	9.34	9.40	9.450	0.1418	9.5	0.5	9.59
30s His	Tyr	4.87	5.02	5.13	5.007	0.1305	5.0	0.5	5.07
30s His	Phe	14.47	15.60	15.28	15.120	0.5866	15.2	1.0	15.28
30s His	Arg	10.44	11.30	10.94	10.900	0.4366	11.0	1.0	11.16
90s His	Tyr	16.06	16.10	15.86	16.010	0.1286	15.8	1.0	15.32
90s His	Phe	4.67	4.60	4.63	4.633	0.0351	4.6	0.5	4.64
90s His	Arg	8.72	8.79	8.50	8.670	0.1513	8.6	0.5	8.48
Glu	Tyr	7.36	7.10	7.13	7.197	0.1422	7.2	0.5	7.24
Glu	Phe	12.17	11.80	11.77	11.900	0.2309	11.9	0.5	11.96
Glu	Arg	6.33	6.16	5.87	6.120	0.2326	6.1	0.5	6.00

Fig. 12/2